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Crystal nucleation and cluster-growth kinetics in a model glass under shear

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Abstract

Crystal nucleation and growth processes induced by an externally applied shear strain in a model metallic glass are studied by means of nonequilibrium molecular dynamics simulations, in a range of temperatures. We observe that the nucleation-growth process takes place after a transient, induction regime. The critical cluster size and the lag-time associated with this induction period are determined from a mean first-passage time analysis. The laws that describe the cluster-growth process are studied as a function of temperature and strain rate. A theoretical model for crystallization kinetics that includes the time dependence for nucleation and cluster growth is developed within the framework of the Kolmogorov-Johnson-Mehl-Avrami scenario and is compared with the molecular dynamics data. Scalings for the cluster-growth laws and for the crystallization kinetics are also proposed and tested. The observed nucleation rates are found to display a nonmonotonic strain rate dependency.

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